Elasticity-Based TSWarp Cost Functions

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September 11, 2003

1 Introduction

The intent of this short note is to compile my ideas for using the existing mathematics and physics of linear elasticity to provide a cost function and deformation basis for the TSWarp project. I do not present a definitive answer; I merely suggest possibilities and provide the necessary framework for further discussion. Once the features of desired warps are determined then the cost function can be constructed quickly. I assume that the reader is familiar with the TSWarp concept and I will not re-invent it here.

Some of the nice features of an elasticity-based warping cost are: the mathematics is fully developed; all connected warps are potentially realizable; and natural distortion basis functions are often available. Possible drawbacks are that a warping cost of elastic energy is linear and often restricted to crystal symmetries.

Section 2 presents the equations of linear elasticity of solids and fluids. This includes all of the notation (without apology), the equations of motion and the elastic energy equations. The concept of normal harmonic modes is presented and discussed in the context of TSWarp. Section 3 provides a descriptive discussion of the elastic constants and solid deformations. Section 4 presents specific solutions for a variety of special cases. For each case I present a formulation for calculated the energy cost function and determining the natural deformation basis. Section 5 addresses the question of using a rectangular TS space to represent a cylindrically symmetric underlying space. Examples are included here also and they are compared to those of the previous section. A final section outlines my recommendations for trial bases and cost functions.

2 Linear Elasticity Equations

The elastic equations are presented here without a lot of derivation, but hopefully with a good amount of discussion and explanation. Everything is written in the usual summation notation (repeated indices indicate sums over their range). All equations utilize cartesian coordinates, which fortunately are a natural for the TSwarp concept.

The strain (relative deformation) for a material is given by a rank 2 tensor

$$\epsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) \tag{1}$$

where the indices range along the three spatial dimensions, u_k is the displacement from equilibrium in the k^{th} direction and $\partial u_k/\partial x_l$ then is the relative displacement in the k^{th} direction moving along the l^{th} direction. Remember that, in general, $u_k = u_k(x_1, x_2, x_3)$. This strain tensor is the symmetric part of the more intuitive tensor $\epsilon_{kl} = \partial u_k/\partial x_l$. The symmetric choice shown above eliminates rigid rotations.

Similarly, the stress (tension) for a material is also a rank 2 tensor σ_{ij}. The stress and stain are connected by a Hooke's Law relationship through a rank 4 tensor:

$$\sigma_{ij} = c_{ijkl}\epsilon_{kl}. \tag{2}$$

This rank 4 tensor c_{ijkl} is the elasticity tensor and is identical in concept to the constant connecting the restoring force and displacement of a simple harmonic oscillator.

It will be important for us to consider the simple harmonic motion of a material of elasticity c_{ijkl}. The equations are

$$\rho\omega^2 u_i + c_{ijkl}u_{k,jl} = 0. \tag{3}$$

The boundary conditions vary among applications and can be quite complex. Two that are of importance (because they are simple) are free boundary conditions

$$n_j\sigma_{ij} = n_j c_{ijkl}u_{k,l} = 0 \tag{4}$$

and fixed boundary conditions

$$n_j u_j = 0. \tag{5}$$

The elasticity tensor has up to 81 values (3^4). Fortunately, the number of independent values can be no greater than 21 due to symmetry constraints (not material constraints). [If the stout at heart wish to closely examine these symmetries, one finds that by considering shear strains we have $c_{ijkl} = c_{ijlk}$, by considering axial strains we have $c_{ijkl} = c_{jikl}$, and by considering centrosymmetry we have $c_{ijkl} = c_{klij}$.]

Because of all of these wonderful symmetries it is possible to reduce the complexity of the notation. This is done by convention using the following index correspondences:

$$11 \to 1 \quad 22 \to 2 \quad 33 \to 3 \quad 23 \to 4 \quad 13 \to 5 \quad 12 \to 6 \tag{6}$$

which allow the stress and strain tensors to be written as matrices with simplified notation:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \rightarrow \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \tag{7}$$

$$\begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} \rightarrow \frac{1}{2} \begin{bmatrix} 2\epsilon_1 \\ 2\epsilon_2 \\ 2\epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix} \tag{8}$$

As a result, the elasticity tensor is also written as a matrix:

$$c_{ijkl} \rightarrow \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{bmatrix} \tag{9}$$

At least now we can write down the elasticity equations in a relatively simple notation. Note, however, that these new matrices are not tensors and they do not transform as tensors. For example, a coordinate transformation on the elasticity must be performed on c_{ijkl} and not on the reduced notation matrix c_{ij}.

Next, I present the energy equations. The infinitesimal work dW done on a solid through a set of small strains $d\epsilon_i$ is

$$dW = \sigma_i d\epsilon_i. \tag{10}$$

Using Eq.2 in reduced notation and integrating, the energy density per unit volume e is found to be

$$e = \frac{1}{2} c_{ij} \epsilon_i \epsilon_j, \tag{11}$$

and the strain energy E of the solid is

$$E = \frac{1}{2} \int_V c_{ij} \epsilon_i \epsilon_j dV. \tag{12}$$

It is this energy that I propose as a warping cost function.

3 Discussion on Elasticity

I will now try and give the reader an intuitive feel for the meaning behind the various elastic constants c_{ij} and the energy cost function E. At times it will be necessary to take brief forays into crystal symmetry.

For clarity, let the three spatial dimensions now be given their application descriptions: the indices $(i, j, etc.)$ can take on the three directions (t, z, r) corresponding to the direction axes of the TSwarp space. Beginning with the strains we have the useful descriptions:

$\epsilon_{tt} = \epsilon_1$	t-dependent deformation in the t direction
$\epsilon_{zz} = \epsilon_2$	z-dependent deformation in the z direction
$\epsilon_{rr} = \epsilon_3$	r-dependent deformation in the r direction
$\epsilon_{zr} = \epsilon_4$	z-dependent deformation in the r direction
$\epsilon_{rt} = \epsilon_5$	r-dependent deformation in the t direction
$\epsilon_{tz} = \epsilon_6$	t-dependent deformation in the z direction

Keep in mind that $\epsilon_{ij} = \epsilon_{ji}$ provides the remaining definitions (inherent in the reduced single-index notation.

Consider ϵ_1. This corresponds to a stretching in the time dimension whose magnitude depends only on the time coordinate value. One can imagine taking a rectangular parallelepiped (RP) and lengthening it into a larger RP.

Consider ϵ_6. This also corresponds to a stretching in the time dimension. But the magnitude depends only on the local z-coordinate value. An ϵ_6 shifts constant-z surfaces in the t-direction.

The remaining four deformation types are identical to those just described but applied to the various axes.

The stresses (tensions) are defined analogously to the strains. So, for all 21 possible elastic constants we have the following descriptions of the Hooke's Law type connections between the stresses and strains:

c_{11} : uniaxial t stress $\Rightarrow$ t extension strain
c_{22} : uniaxial z stress $\Rightarrow$ z extension strain
c_{33} : uniaxial r stress $\Rightarrow$ r extension strain
c_{44} : z-dep r shear stress $\Rightarrow$ z-dep r shear strain
c_{55} : r-dep t shear stress $\Rightarrow$ r-dep t shear strain
c_{66} : t-dep z shear stress $\Rightarrow$ t-dep z shear strain
c_{12} : uniaxial z stress $\Rightarrow$ t extension strain
c_{13} : uniaxial r stress $\Rightarrow$ t extension strain
c_{23} : uniaxial r stress $\Rightarrow$ z extension strain
c_{14} : z-dep r shear stress $\Rightarrow$ t extension strain
c_{15} : r-dep t shear stress $\Rightarrow$ t extension strain
c_{16} : t-dep z shear stress $\Rightarrow$ t extension strain
c_{24} : z-dep r shear stress $\Rightarrow$ z extension strain
c_{25} : r-dep t shear stress $\Rightarrow$ z extension strain
c_{26} : t-dep z shear stress $\Rightarrow$ z extension strain
c_{34} : z-dep r shear stress $\Rightarrow$ r extension strain
c_{35} : r-dep t shear stress $\Rightarrow$ r extension strain
c_{36} : t-dep z shear stress $\Rightarrow$ r extension strain
c_{45} : r-dep t shear stress $\Rightarrow$ z-dep r shear strain
c_{46} : t-dep z shear stress $\Rightarrow$ z-dep r shear strain
c_{56} : t-dep z shear stress $\Rightarrow$ r-dep t shear strain

For example, $c_{12} > 0$ means that a stretching in the z-direction will produce an axial tension in the t-direction. With free boundary conditions this means the material will expand in the t-direction. Similarly, if $c_{12} < 0$ the material will contract in the t-direction under the same conditions.

Consider $c_{16} \neq 0$. This term shows that a z-direction shear dependent on the time coordinate (displacing the equal time surfaces in the z-direction) produces an axial tension in the t-direction! This example seems to be unrealistic, but this situation is possible when one considers molecular orientation effects in real crystals.

Consider $c_{56} \neq 0$. The same shear as just described can now also produce a t shear of r-dependence. This effect also can only be due to molecular orientation effects.

The possibilities are rich indeed. All 21 coefficients can be independent; indeed they are for triclinic crystals. The various physically realizable crystal symmetries have varying number of independent coefficients (not all combinations are allowed!). But even an isotropic material is nontrivial with two independent coefficients: $c_{11} = c_{22} = c_{33}, c_{12} = c_{13} = c_{23}$, and $c_{44} = c_{55} = c_{66} = (c_{11} - c_{12})/2$. They are also related to the (possibly more familiar) Lamé parameters: $\lambda = c_{11}, \mu = c_{44}$ and Poisson's ratio $\sigma = c_{11}/2(c_{11} + c_{44})$.

The entire c_{ij} description is given here because it is not obvious to me which terms might be more or less important for the TSWarp application. The presence of nonzero terms can only be decided on the basis of the underlying physics of the problem – a topic which is beyond the scope of this note.

4 Cost Functions and Deformation Bases

In this section I present several cost function possibilities based upon resolvable cases of Eq. 3. The cost functions are accompanied by a natural basis set describing the deformation.

4.1 Anisotropic Fluid

Yes, so far as I am aware, there isn't any such material as an anisotropic fluid. Nevertheless, the mathematics does not suffer and this material description may be the simplest nontrivial solution to the TSwarp cost function. A fluid has no shear components to the stresses or strains. So only three elasticity components are needed to describe the behavior: c_{11}, c_{22}, and c_{33}. If these constants are allowed to be independent then we have our anisotropy.

For this simple system the normal modes and energies of harmonic motion can be computed. Then, if an arbitrary warp is described as a sum of normal mode amplitudes then the problem of calculating the cost function is solved. The derivation proceeds as follows.

A fluid of constant vorticity is described by a velocity potential function Φ:

$$\vec{v} = -\vec{\nabla}\Phi; \qquad p = \rho\frac{\partial\Phi}{\partial\tau} \tag{13}$$

Here I use τ to indicate wave motion time to avoid confusion with the TSWarp time t. For simple harmonic motion, the wave equation becomes

$$\nabla^2\Phi + k^2\Phi = 0 \tag{14}$$

where k is the ratio of the harmonic frequency to the wave velocity $k = \omega/c$. For the TSWarp project $\Phi = \Phi(z, r, t)$. I first consider the boundary conditions to be free at all surfaces except at $r = 0$ where rigid boundary conditions will be enforced:

$$\begin{aligned} v_r &= 0 \quad \text{at } r = 0 \\ \tfrac{\partial\Phi}{\partial\tau} &= 0 \quad \text{otherwise at boundaries} \end{aligned} \tag{15}$$

I am using the idea that the velocity field is equivalent to the displacement field modulo a time shift. The spatial amplitude of the velocity and displacement are proportional. Thus, either is descriptive of the desired eigenmode basis. Now, the wave equation

$$\left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial r^2} + \frac{\partial^2}{\partial t^2}\right)\Phi + k^2\Phi = 0 \tag{16}$$

is easily solved using the standard method of separation of variables:

$$\begin{aligned} \Phi &= f(z)g(r)h(t) \\ f(z) &= \alpha_z sin(k_z z) + \beta_z cos(k_z z) \\ g(r) &= \alpha_r sin(k_r r) + \beta_r cos(k_r r) \\ h(t) &= \alpha_\tau sin(k_t t) + \beta_t cos(k_t t). \end{aligned} \tag{17}$$

Applying the boundary conditions on the intervals $0 \leq z \leq b$, $0 \leq r \leq c$ and $0 \leq t \leq c$ yields the velocity potential functions

$$\Phi_\lambda = \Phi_{\lambda,0} sin\left(\frac{m\pi t}{a}\right) sin\left(\frac{n\pi z}{b}\right) sin\left(\frac{(2p-1)\,\pi r}{2c}\right) \tag{18}$$

where λ indexes the positive integer triplet (m, n, p) that identifies the mode. The displacement vector is determined from $\partial\vec{u}_\lambda/\partial\tau = -\vec{\nabla}\Phi_\lambda$:

$$\begin{aligned}\vec{u}_\lambda = N_\lambda \quad & \left[\tfrac{m\pi}{a} cos\left(\tfrac{m\pi t}{a}\right) sin\left(\tfrac{n\pi z}{b}\right) cos\left(\tfrac{(2p-1)\pi r}{2c}\right)\hat{t}\right. \\ & +\tfrac{n\pi}{b} sin\left(\tfrac{m\pi t}{a}\right) cos\left(\tfrac{n\pi z}{b}\right) cos\left(\tfrac{(2p-1)\pi r}{2c}\right)\hat{z} \\ & \left.-\tfrac{(2p-1)\pi}{2c} sin\left(\tfrac{m\pi t}{a}\right) sin\left(\tfrac{n\pi z}{b}\right) sin\left(\tfrac{(2p-1)\pi r}{2c}\right)\hat{r}\right]\end{aligned} \tag{19}$$

A volume normalization

$$\int_V \vec{u}_\lambda \vec{u}_{\lambda'} dV = \delta_{\lambda,\lambda'} \tag{20}$$

yields the mode-dependent normalization factor

$$N_\lambda = \left(\frac{8}{abc\pi^2}\right)^{1/2} \left(\frac{m^2}{a^2} + \frac{n^2}{b^2} + \frac{(2p-1)^2}{(2c)^2}\right)^{-1/2}. \tag{21}$$

Continuing this example, the energy density, Eq. 11, is given by:

$$e_\lambda = \frac{1}{2}\left[c_{11}\epsilon_1^2 + c_{22}\epsilon_2^2 + c_{33}\epsilon_3^2\right], \tag{22}$$

$$e_\lambda = \frac{1}{2}c_{11}\left[\frac{\partial}{\partial t}\left(\vec{u}_\lambda \cdot \hat{t}\right)\right]^2 + \frac{1}{2}c_{22}\left[\frac{\partial}{\partial z}\left(\vec{u}_\lambda \cdot \hat{z}\right)\right]^2 + \frac{1}{2}c_{33}\left[\frac{\partial}{\partial r}\left(\vec{u}_\lambda \cdot \hat{r}\right)\right]^2. \tag{23}$$

The total energy in a given mode is the integral of Eq. 23 over the volume of the fluid. It is

$$E_\lambda = \left(\frac{\pi}{2}\right)^4 abcN_\lambda^2 \left[c_{11}\left(\frac{m}{a}\right)^4 + c_{22}\left(\frac{n}{b}\right)^4 + c_{33}\left(\frac{(2p-1)}{2c}\right)^4\right] \tag{24}$$

A given arbitrary small warping is represented by $\vec{u} = \alpha_\lambda \vec{u}_\lambda$ and the total energy is

$$E = \alpha_\lambda^2 E_\lambda \tag{25}$$

where repeated indices indicate summation over all possibilities.

Here is an example of a cost function (Eq. 25) that is easy to compute given the anisotropic fluid deformation basis (Eq. 19). It is possible to choose a finite basis set that emphasizes some directions over others by either limiting the maximum utilized (m, n, p) or by suitable choices of the elastic coefficients. The potential of the latter is more fully explored in the section on RUS solids.

Alterations in the boundary conditions are not transparent to either the basis functions or to the energy. For example, if a fixed boundary is imposed at $r = c$ as well as at $r = 0$ then $g(r) = \beta_r cos(p\pi/c)$ and $(p - 1/2) \rightarrow p$ in all other equations.

It may take extra thought and some work to establish the best deformation basis. The anisotropic fluid model is quite simple. Potential pitfalls are that it does not contain pure shear deformations and it cannot easily accommodate mixed boundary conditions. So, it may be revealed through testing that this model is not sufficient to describe necessary warps. On the other hand, a perfect basis may not be necessary. It is sufficient that the warping cost forces the simulation parameterization to converge to a zero-warp state.

4.2 Fluid

An isotropic fluid (the kind that really exists on planet Earth) is described by the equations in the previous section with the one modification that $c_{11} = c_{22} = c_{33}$. In fact, c_{11} is the bulk modulus K of the fluid:

$$c_{11} = K = -V\frac{\partial p}{\partial V}. \tag{26}$$

The cost function is

$$E_\lambda = \left(\frac{\pi^2 K}{2}\right) \frac{\left(\frac{m}{a}\right)^4 + \left(\frac{n}{b}\right)^4 + \left(\frac{(2p-1)}{2c}\right)^4}{\left(\frac{m}{a}\right)^2 + \left(\frac{n}{b}\right)^2 + \left(\frac{(2p-1)}{2c}\right)^2} \tag{27}$$

This energy is not much simpler than for the anisotropic fluid and includes the loss of generality in choosing elastic constants.

4.3 Isotropic Solid

The simplest possible physically realizable solid material is one that is isotropic. Two elastic constants are all that are needed to describe the stress-strain behavior: one for compressional effects and one for shear effects. The relationships are $c_{11} = c_{22} = c_{33}$, $c_{12} = c_{13} = c_{23}$, and $c_{44} = c_{55} = c_{66} = (1/2)(c_{11} - c_{12})$ as well as all related equivalences. The equations of harmonic motion show that even this solid is not quite so simple as one might wish. The coupled equations of motion are:

$$\begin{aligned}
-2\rho\omega^2 u_1 = \;& c_{11}\left(2u_{1,11} + u_{1,33} + u_{1,22}\right) \\
& + c_{12}\left(2u_{2,12} + 2u_{1,21} + 2u_{3,13} + 2u_{1,31} - u_{1,33} - u_{1,22}\right) \\
-2\rho\omega^2 u_2 = \;& c_{11}\left(2u_{2,22} + u_{2,11} + u_{2,33}\right) \\
& + c_{12}\left(2u_{3,23} + 2u_{2,32} + 2u_{1,21} + 2u_{2,12} - u_{2,11} - u_{2,33}\right) \\
-2\rho\omega^2 u_3 = \;& c_{11}\left(2u_{3,33} + u_{3,22} + u_{3,11}\right) \\
& + c_{12}\left(2u_{1,31} + 2u_{3,13} + 2u_{2,32} + 2u_{3,23} - u_{3,22} - u_{3,11}\right)
\end{aligned} \tag{28}$$

These equations are nontrivial and I am not aware of analytical solutions, nor have I searched for any. Even in some simple cases no analytic solutions exists (e.g. sphere, thin

rod). It seems unlikely that a two-parameter isotropic solid solution would perform much better as a cost function to the three parameter anisotropic fluid solution. Nevertheless, an accurate numerical solution can be obtained using the RUS method described in the next section.

Equations 28 hint at the potential complexity in describing the motion (or energy density) in real solids. The complexity is only defeated by numerical computation and/or approximating methods.

4.4 RUS Solids

Resonant Ultrasound Spectroscopy (RUS) is an experimental technique for determining the elastic constants of a solid from low frequency normal mode resonances. The mathematical structure can be adapted for use in computing the warping cost function and low-frequency normal mode shapes. The method is general to all homogeneous solids, but is not practical for all from a computational time standpoint. The solution is numerically calculated. Given a set of elastic constants, the outputs are the resonance frequencies below a cutoff frequency and the corresponding eigenfunctions. But, the solid must have free boundary conditions.

Here is a summary of the mathematics. The Lagrangian for the motion of an elastic solid is

$$L = \int_V (KE - PE)\, dV \tag{29}$$

$$L = \frac{1}{2} \int_V \left(\rho \omega^2 u_i u_i - c_{ijkl} u_{i,j} u_{k,l} \right) dV. \tag{30}$$

Variational minimization yields

$$\delta L = \int_V \left(\rho \omega^2 u_i \delta u_i + c_{ijkl} u_{k,jl} \delta u_i \right) dV - \int_S \left(\vec{n}_j c_{ijkl} u_{k,l} \delta u_i \right) dS \tag{31}$$

Since the variation must be independent of δu_i the volume term of Eq. 31 yields the harmonic equation of motion (Eq. 3), and the surface term yields the free boundary condition (Eq. 4).

Now, expand the displacement vector in a complete (not necessarily orthonormal) set of functions ϕ_λ:

$$u_i = a_{i\lambda} \phi_\lambda \tag{32}$$

Then the Lagrangian takes on the form

$$L = \frac{1}{2} \int_V \left(\delta_{ii'} \rho \omega^2 a_{i\lambda} a_{i'\lambda'} \phi_\lambda \phi_{\lambda'} - c_{ijkl} a_{i\lambda} a_{i'\lambda'} \phi_{\lambda,j} \phi_{\lambda',l} \right) dV. \tag{33}$$

If $\vec{a}$ is written as a column vector with elements ranging over i and λ, then we can define also the two matrices:

$$A_{i\lambda i'\lambda'} = \delta_{ii'} \int_V \phi_\lambda \rho \phi_{\lambda'} dV, \tag{34}$$

and

$$B_{i\lambda i'\lambda'} = c_{iji'j'} \int_V \phi_{\lambda,j} \phi_{\lambda',j'} dV, \tag{35}$$

These matrices are square with row indices running over i and λ and column indices running over i' and λ'. These representations simplify the Lagrangian considerably:

$$L = \frac{1}{2} \left(\omega^2 \vec{a}^T A \vec{a} - \vec{a}^T B \vec{a} \right). \tag{36}$$

But, better yet, if the Lagrangian is stationary with respect to the amplitudes $a_{i\lambda}$ then the displacements u_i are a solution to the free vibration problem, and from Eq. 36 the eigenvalue equation is:

$$\omega^2 A \vec{a} = B \vec{a}. \tag{37}$$

The solution to this eigenvalue equation equation yields the eigenvectors which are exactly the normal mode displacement basis. In order to accomplish this, the function set ϕ_λ must be finite as well as small enough to be practical computationally. For RUS applications A useful expansion function set is

$$\phi_\lambda = x^f y^g z^h \tag{38}$$

where λ indexes the possible positive triplets (f, g, h) such that the truncation condition $f+g+h \leq N$ is satisfied. This choice of ϕ_λ allows the direct and analytic computation of the matrices A and B. This function set has been shown to work well for many materials with non-simple convex boundaries. For the RP of TSWarp a different basis set may be more desirable. For example, one might choose an orthonormal set from the functions shown in section 4.1 with a similar truncation condition $m + n + p \leq N$. Note that this is not a set of normal modes – it is the expansion set by which the normal modes can be approximated.

Next, consider the calculation of the strain energy for a given displacement vector. There are some complications because of the expansion basis formalism. For a given N the Rank R of the matrices A and B is $R = (N+1)(N+2)(N+3)/2$. If $N \to \infty$ then the solutions are 'exact'. But for computational purposes we must keep N rather small. In addition, only the lowest frequency eigenmodes of the computable R modes can be expected to be accurate. Experience with RUS has shown that N=10 is sufficient to accurately compute the first 50 or so eigenmodes in a RP solid of three comparable dimensions.

The actual computation begins with the calculation of the M lowest frequency eigenmodes $\vec{w}_i$ using Eq. 37:

$$\vec{w}_i \qquad i = 1, 2, ..., M << R. \tag{39}$$

The energy for each eigenmode is then computed for unit amplitude:

$$E_i = \frac{1}{2}\omega_i^2 \vec{w_i}^T A \vec{w_i} + \frac{1}{2}\vec{w_i}^T B \vec{w_i}, \tag{40}$$

$$E_i = \vec{w_i}^T B \vec{w_i}, \tag{41}$$

$$E_i = \omega_i^2 \vec{w_i}^T A \vec{w_i}. \tag{42}$$

A displacement (warping) $\vec{u}$ is written as an expansion in the eigenmodes with coefficients α_i.

$$\vec{u} = \alpha_i \vec{w_i}. \tag{43}$$

Then the total energy cost function is:

$$E = \vec{u}^T B \vec{u} = \alpha_i^2 E_i. \tag{44}$$

The eigenmode energies are computed once from Eq. 41 or Eq. 42, both of which require the solution of the eigenvalue equation (Eq. 37). The warping cost for each test warp (Eq. 33) is then quickly computed using Eq. 44. The previous examples (high degree of symmetry cases) are clearly special cases of this formulation.

One attractive feature of the RUS-based normal mode approach is that it provides all of the modes that have energies below a cutoff energy and ignores all others. Thus, by suitable choice of elastic constants, it is possible to concentrate warping along certain directions or among certain mode types. For example, choosing a large c_{11} (relative to other coefficients) guarantees that extensional modes in the 1-direction will be fewer in number than for other directions. One can also concentrate on shear modes by making the material very stiff toward extensional deformations. The possibilities are many, and the RUS formalism provides this benefit without any additional work.

It is not clear to me how this approach can be generalized to include fixed or mixed boundary conditions.

4.5 Generalized Approach

The strain energy of a solid is independent of the choice of functions describing the stress. Thus, one can use Eq. 12 and compute the integral directly for any choice of basis functions and boundary conditions. Two cautions come to mind. First, care must be taken to choose an orthogonal basis. Second, it is often not clear how to obtain a complete basis.

This approach is no more computationally costly than any of the previous methods. One calculates the energies E_i associated with the basis functions w_i, expands the warping in terms of this basis (Eq. 43), then computes the total energy according to Eq, 44.

As an example, choose basis functions found for the anisotropic fluid (Eq. 19 in Section 4.1 (thus imposing the same boundary conditions given by Eq. 15) and apply them to the general formulation requiring 21 independent elastic constants. All other symmetries will then be specific reductions of this result.

The energy is computed using the same approach outlined in Section 4.1 with care taken to include all terms of Eq. equ:equ11. The result is

$$\begin{aligned} E_\lambda = \tfrac{1}{(\bar{m}^2+\bar{n}^2+\bar{p}^2)} \quad & \left[\tfrac{1}{2}c_{11}\bar{m}^4 + \tfrac{1}{2}c_{22}\bar{n}^4 + \tfrac{1}{2}c_{33}\bar{p}^4\right. \\ & + \left(\tfrac{1}{2}c_{44} + c_{12}\right)\bar{m}^2\bar{n}^2 + \left(\tfrac{1}{2}c_{55} + c_{13}\right)\bar{m}^2\bar{p}^2 + \left(\tfrac{1}{2}c_{66} + c_{23}\right)\bar{n}^2\bar{p}^2 \\ & + c_{14}\bar{m}^3\bar{n} + c_{15}\bar{m}^3\bar{p} + c_{24}\bar{n}^3\bar{m} + c_{26}\bar{n}^3\bar{p} + c_{35}\bar{p}^3\bar{m} + c_{36}\bar{p}^3\bar{n} \\ & \left. + \left(c_{16} + c_{45}\right)\bar{m}^2\bar{n}\bar{p} + \left(c_{25} + c_{46}\right)\bar{m}\bar{n}^2\bar{p} + \left(c_{34} + c_{56}\right)\bar{m}\bar{n}\bar{p}^2\right] \end{aligned} \tag{45}$$

where I use the simplified mode index notation:

$$\begin{aligned} \bar{m} &= \left(\tfrac{m\pi}{a}\right) \\ \bar{n} &= \left(\tfrac{n\pi}{b}\right) \\ \bar{p} &= \left(\tfrac{(2p-1)\pi}{2c}\right) \end{aligned} \tag{46}$$

These energies are easily tabulated and the eigenfunctions are simple to apply. The total energy for a displacement $\vec{u}$ is given by Eq. 25.

The fluid results of sections 4.1 and 4.2 follow directly from Eq. 46 under the appropriate limiting cases for the c_{ij}.

This generalized approach may not be the not be the most clever, nor is it necessarily the most descriptive of an elastic solid. But it is probably the easiest nontrivial approach to getting a cost function and deformation basis. The warping basis chosen for this example is not complete. I have ignored the entire set of pure shear modes.

5 Application to Cylindrical Spatial Coordinates

This section begins with a quote of a previous discussion about using cylindrical spatial coordinates followed by a 4D calculation example analogous to that of Section 4.5.

5.1 Previous 4D Discussion

This section addresses the challenge of using a cartesian coordinate basis to describe an underlying time-space dynamics in cylindrical symmetry. Since the warping is applied in the radiograph space we expect symmetry about the line $r = 0$. We must be careful to not under-emphasize the effects of warping regions of large r relative to the central regions. For the simulation space is dominated by large r.

One possible solution is to perform a transformation on the radiograph space from $r \to r^2$ prior to warping followed by the inverse transformation. However, this would seem to emphasize distortions at large r rather than emphasize importance or cost. It amounts to a somewhat unusual change of basis functions.

Another possible solution is to apply position dependent elasticity. In this case, I believe that the energy equation (Eq. 12) still holds. The resulting calculation of the energies of the basis functions is more complicated, but otherwise we have no theoretical

changes. Consider the case of the anisotropic fluid with $c_{33} \rightarrow c_{33} + \beta r^2$. We suppose that Eq. 23 still holds and integrate over the solid to obtain Eq. 24 altered only by $\epsilon_{33} \rightarrow \epsilon_{33} + \beta\frac{c^2}{12}$. Even this approach yields only an effective increase in some elastic constants. This is a direct result of our choice of basis functions. We might then choose a basis with amplitude dependence on r. But I don't know what this basis might be.

5.2 Generalized Approach in 4D

Now I would like to present a cylindrical solution formulated in 4D – three spatial dimensions and one time dimension. The cylindrical symmetry will bring it back to 3D but only in 4D do we find the correct eigenfunctions and energies. I begin with the fluid motion basis set and apply it to the general formulation. Begin with the wave equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 \Phi}{\partial \phi^2} + \frac{\partial^2 \Phi}{\partial z^2} + \frac{\partial^2 \Phi}{\partial t^2} + k^2\Phi = 0, \tag{47}$$

and invoke our assumption that Φ is independent of the azimuthal coordinate ϕ:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Phi}{\partial r}\right) + \frac{\partial^2 \Phi}{\partial z^2} + \frac{\partial^2 \Phi}{\partial t^2} + k^2\Phi = 0. \tag{48}$$

Again using separation of variables, we let $\Phi(r, z, t) = f(z)g(r)h(t)$. For definiteness I impose free boundary conditions on the surfaces with normals in the $\hat{z}$ and $\hat{t}$ directions, obtaining

$$\begin{aligned} f(z) &\propto sin\left(\tfrac{n\pi z}{b}\right) \\ h(t) &\propto sin\left(\tfrac{m\pi t}{a}\right). \end{aligned} \tag{49}$$

The remaining radial equation is thus,

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}g(r)\right) + \left[k^2 - \left(\frac{n\pi}{b}\right)^2 - \left(\frac{m\pi}{a}\right)^2\right] g(r) = 0. \tag{50}$$

This is the cylindrical Bessel's Equation with solution

$$g(r) \propto J_0(\bar{k}r) \tag{51}$$

where $J_0(\cdot)$ is the zeroth order cylindrical Bessel Function and

$$\bar{k}^2 \equiv k^2 - \left(\frac{n\pi}{b}\right)^2 - \left(\frac{m\pi}{a}\right)^2. \tag{52}$$

A fixed boundary at $r = c$ requires that

$$J_0'(\bar{k}c) = 0; \qquad \bar{k} \equiv \frac{\alpha_p}{c} \tag{53}$$

where α_p is the p_{th} root of $J_0'(x) = 0$. A free boundary at $r = c$ requires that

$$J_0(\bar{k}c) = 0; \qquad \bar{k} \equiv \frac{\beta_p}{c} \tag{54}$$

where β_p is the p_{th} root of $J_0(x) = 0$. Thus, both simple boundary conditions are readily formulated. I continue here with the free boundary condition case, so that

$$k^2 = \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 + \left(\frac{\beta_p}{c}\right)^2 \tag{55}$$

and the velocity potential is

$$\Phi_\lambda = \Phi_{\lambda,0} sin\left(\frac{m\pi t}{a}\right) sin\left(\frac{n\pi z}{b}\right) J_0\left(\frac{\beta_p r}{c}\right) \tag{56}$$

where λ indexes the positive integer triplets (m, n, p) as usual. The displacement eigenmodes are (following the approach taken in computing Eq. 19:

$$\begin{aligned} \vec{u}_\lambda = M_\lambda \quad & \left[\tfrac{m\pi}{a} cos\left(\tfrac{m\pi t}{a}\right) sin\left(\tfrac{n\pi z}{b}\right) J_0\left(\tfrac{\beta_p r}{c}\right) \hat{t}\right. \\ & + \tfrac{n\pi}{b} sin\left(\tfrac{m\pi t}{a}\right) cos\left(\tfrac{n\pi z}{b}\right) J_0\left(\tfrac{\beta_p r}{c}\right) \hat{z} \\ & \left. - \tfrac{\beta_p}{c} sin\left(\tfrac{m\pi t}{a}\right) sin\left(\tfrac{n\pi z}{b}\right) J_1\left(\tfrac{\beta_p r}{c}\right) \hat{r}\right] \end{aligned} \tag{57}$$

The normalization factor M_λ is calculated using the volume normalization

$$\int_V \left(\vec{u}_{\lambda_1} \cdot \vec{u}_{\lambda_2}\right) r dr d\phi dz dt = \delta_{\lambda_1,\lambda_2}. \tag{58}$$

Now, skipping a lot of steps, I find the normalization factor to be

$$M_\lambda^2 = \frac{8}{2\pi abc^2 J_1^2(\beta_p)} \left[\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 + \left(\frac{\beta_p}{c}\right)^2\right]^{-1}. \tag{59}$$

For future reference, I used Eq. 54 and the identity $xJ_1'(x) = xJ_0(x) - J_1(x)$ in the derivation. The energy density is calculated according to Eq. 23 noting that there is no remaining ϕ-dependence. I make use also of the following two relations:

$$\int_0^c J_0^2\left(\frac{\beta_p r}{c}\right) r dr = \frac{c^2}{2} J_1^2\left(\beta_p\right), \tag{60}$$

and

$$I \equiv \frac{2\int_0^c \left[J_1'\left(\frac{\beta_p r}{c}\right)\right]^2 r dr}{\beta_p^2 J_1^2\left(\beta_p\right)}. \tag{61}$$

I do not know of a non-integral expression for the quantity I, but it can be computed numerically to any desired accuracy. For the anisotropic fluid, the total deformation energy per mode is

$$E_\lambda = \frac{\frac{1}{2}c_{11}\hat{m}^4 + \frac{1}{2}c_{22}\hat{n}^4 + \frac{1}{2}c_{33}\hat{p}^4}{\hat{m}^2 + \hat{n}^2 + \hat{p}^2} \tag{62}$$

where I have defined three new mode index notation parameters:

$$\begin{aligned}\hat{m} &= \bar{m} = \left(\tfrac{m\pi}{a}\right) \\ \hat{n} &= \bar{n} = \left(\tfrac{n\pi}{b}\right) \\ \hat{p} &= \sqrt{I}\left(\tfrac{\beta_p}{c}\right)\end{aligned} \tag{63}$$

The 4D result for an arbitrary set of elastic constants, using the incomplete basis set Eq. 57, is Eq. 45 with the replacement $\bar{p} \to \hat{p}$. I will reproduce it here for reference purposes.

$$\begin{aligned}E_\lambda = \tfrac{1}{(\hat{m}^2+\hat{n}^2+\hat{p}^2)} \quad & \left[\tfrac{1}{2}c_{11}\hat{m}^4 + \tfrac{1}{2}c_{22}\hat{n}^4 + \tfrac{1}{2}c_{33}\hat{p}^4\right. \\ & + \left(\tfrac{1}{2}c_{44} + c_{12}\right)\hat{m}^2\hat{n}^2 + \left(\tfrac{1}{2}c_{55} + c_{13}\right)\hat{m}^2\hat{p}^2 + \left(\tfrac{1}{2}c_{66} + c_{23}\right)\hat{n}^2\hat{p}^2 \\ & + c_{14}\hat{m}^3\hat{n} + c_{15}\hat{m}^3\hat{p} + c_{24}\hat{n}^3\hat{m} + c_{26}\hat{n}^3\hat{p} + c_{35}\hat{p}^3\hat{m} + c_{36}\hat{p}^3\hat{n} \\ & \left. + \left(c_{16} + c_{45}\right)\hat{m}^2\hat{n}\hat{p} + \left(c_{25} + c_{46}\right)\hat{m}\hat{n}^2\hat{p} + \left(c_{34} + c_{56}\right)\hat{m}\hat{n}\hat{p}^2\right]\end{aligned} \tag{64}$$

6 Recommendations

Based on this study of elasticity-based cost functions for TSWarp, I recommend the following ordered list of approaches. The list suggests beginning with simple implementation with less descriptive bases and works toward more involved implementations using complete bases of real solids. I suggest this order only because my impression is that the simpler approaches stand a very good chance of working.

1. Utilize the deformation basis Eq. 57 and the three-parameter cost function Eq. 62. This is the result of a 4D TSWarp-space calculation for an anisotropic fluid.

2. Utilize the deformation basis Eq. 57 and the multi-parameter cost function Eq. 64. The underlying physics of the problem can be used to suggest which elastic coefficients should be nonzero. This choice may also be evident in studying the ways is which the first approach fails (if it does).

3. Impose all free boundary conditions in 3D TSWarp allowing the radial coordinate the range $[-c, c]$. Apply the RUS calculation to determine a set of basis deformations and energies based on some knowledge of the expected elastic coefficients. Begin with the simplest crystal symmetries and choose more complicated ones as needed.

4. If all of the above methods have failed then I will return to the 4D generalized approach with a more inclusive deformation basis set.